



JOB DESCRIPTION

Job Title : 18-month postdoc position in Quantum Chemistry

Job Summary :
(English, max 1000 characters)

The selected applicant will contribute to the development of new approaches in the field of ensemble density-functional theory for excited states.

Job Description :
(English, detailed information – max 3000 characters)

WARNING: Please indicate the name of the research lab, group leader and supervisor.

The selected applicant will join the “Laboratoire de Chimie Quantique” team (lead by Prof. V. Robert) in the Institute of Chemistry, Unistra, Strasbourg. She/He will be supervised by Prof. E. Fromager.

Density-functional theory (DFT) for ensembles [1] has attracted an increasing attention over the last few years as a potential lower-cost and in-principle-exact alternative to the ubiquitous time-dependent linear response DFT (TD-DFT) formalism for the computation of electronically excited states in situations where TD-DFT fails. We can mention, for example, the description of photochemical processes where energy crossings occur, thus making the linear response regime inadequate. The challenge in ensemble DFT (eDFT) lies in the development of systematically improvable density-functional approximations (DFAs) [2]. For that purpose, we propose to explore two new and complementary strategies: i) an (approximate) evaluation of ground- and excited-state energies from regular (ground-state) DFAs and individual beyond-Kohn-Sham densities, thus providing a (partial) description of density-driven correlation effects [2,3], and ii) a complementary multi-reference perturbation theory treatment (based on the Kohn-Sham ensemble) for the description of state-driven correlation effects [2] as well as response properties such as transition densities, thus allowing for the computation of non-adiabatic couplings, for example.

[1] E.K.U. Gross, L.N. Oliveira, W. Kohn, Phys. Rev. A 37, 2809 (1988).

[2] F. Cernatic, B. Senjean, V. Robert, and E. Fromager, arXiv:2109.04943 (2021).

[3] E. Fromager, Phys. Rev. Lett. 124, 243001 (2020).

Main research field :

WARNING: Please select, trying to be specific, using 'Other' or 'All' will decrease your Job Vacancy visibility

Chemistry/Physics

Offer Requirements :

Eligibility criteria : PhD in quantum chemistry or condensed matter physics, experience in theory development highly appreciated.

JOB DETAIL

Type of contract : time-limited
Status : postdoc
Company / Institute : Université de Strasbourg, Institut de Chimie de Strasbourg
Country : France
City : Strasbourg
Postal Code : 67000
Street : 4 rue Blaise Pascal

APPLICATION DETAILS (mandatory)

Provisional start date : 01/07/2022
Application deadline : 01/03/2022
Application e-mail : fromagere@unistra.fr